MITReM library

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1 Equations and nomenclature

1.1 Stationary mass conservation

$$-\vec{\nabla}.\vec{N}_i + R_i = 0$$

with

$$\vec{N}_i = c_i\vec{v} - \sum_j D_{ij}\vec{\nabla}c_j - w_i c_i \vec{\nabla}U$$

- D_{ij} is the diffusion factor.
- $w_i c_i$ is the migration factor.

1.2 Electrostatics

$$\vec{\nabla}^2 U + \frac{F}{\epsilon}\sum_i z_i c_i = 0$$

- The electrostatics potential factor is 1 if you use Poisson and 0 if you use electroneutrality.
- $\frac{z_i F}{\epsilon}$ is the electrostatics concentration factor if you use Poison and z_i if you use electroneutrality.

1.3 Butler-Volmer kinetics

$$v = k_{ox}\exp\left[\frac{\alpha_{ox}nF}{RT}(V-U)\right]c_{red} - k_{red}\exp\left[-\frac{\alpha_{red}nF}{RT}(V-U)\right]c_{ox}$$

2 Include

Additional Include Directories: MITReM\include
In your code: #include "MITReM.h"

3 Functions

3.1 Constructor

Pass the name of the MITReM files. The constructor will then read all necessary parameters from the name.elecreactions, name.electrolytesolution, name.homreactions and name.models file.

3.2 getNIons()

Returns the number of ions.

3.3 getIonInletConcentrations(i)

Returns the equilibrium concentration of ion i to be imposed on the inlet.

3.4 getNElecReactions()

Returns the number of electrochemical reactions to choose from. Every electrode will have some (or all) of these reactions occuring on its surface.

3.5 getElecReactionLabel(r)

Returns the label of electrochemical reaction r. Use this function to construct the list of indices of electrochemical reactions occuring on the electrode. This list you will have to pass to calcBoundaryElementVec and calcBoundaryElementJac of the ElementMatrixAssembler.